

Sum of squares representation for the Böttcher-Wenzel biquadratic form

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Abstract. We find the minimum scale factor, for which the nonnegative Böttcher-Wenzel biquadratic form becomes a sum of squares (sos). To this we give the primal and dual solutions for the underlying semi-definite program. Moreover, for special matrix classes (tridiagonal, backward tridiagonal and cyclic Hankel matrices) we show that the above form is sos. Finally, we conjecture sos representability for Toeplitz matrices.

1 Introduction

The Böttcher-Wenzel inequality ([1], [2], [3], [7], [6]) states that for real square matrices P, Q the biquadratic form

$$BW \equiv 2 \left(\|P\|^2 \|Q\|^2 - \text{trace}^2(P^T Q) \right) - \|PQ - QP\|^2 \quad (1)$$

is nonnegative, with the Frobenius norm used. Replacing the factor 2 by $2 + \gamma_n$, it is natural to ask for the minimum γ_n such that

$$(2 + \gamma_n) \left(\|P\|^2 \|Q\|^2 - \text{trace}^2(P^T Q) \right) - \|PQ - QP\|^2$$

is a sum of (polynomial) squares. We answer this question in Theorem 1 by showing that the minimum value is $(n - 2)/2$.

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For simplicity, we use one-subscript notation for the entries of P and Q , described by means of the "small" index matrix

$$\text{IND} = ((i-1)n + j)_{i,j=1}^n.$$

Then P and Q can be generated by vectors p and q of dimension $m = n^2$ as

$$P(i, j) = p(\text{IND}(i, j)), \quad 1 \leq i \leq j \leq n.$$

Introducing an index matrix will be especially useful in Sections 3 to 5, where tridiagonal, backward tridiagonal, cyclic Hankel and general Toeplitz matrices will be investigated. For these special cases we prove (for Toeplitz matrices: conjecture) that the corresponding BW form is a sum of squares (sos).

It is quite odd that although (real) Hankel matrices are symmetric, thus normal, hence nonnegativity easily follows [1], this does not imply that a sos form also exists (except if $n = 3$, Example 9). On the other hand, Toeplitz matrices are usually not normal, yet the corresponding BW form is sos, at least according to our well-grounded Conjecture 15 at the end of the paper.

2 The case of general matrices

Let P, Q be arbitrary $n \times n$ real matrices with entries

$$P = (p_{(i-1)n+j})_{i,j}^n, \quad Q = (q_{(i-1)n+j})_{i,j}^n,$$

as indicated above. (Notice that we use this indexing technique for simplicity.) It turns out [5] that the above forms depend only on the variables

$$z_{i,j} = p_i q_j - q_i p_j, \quad 1 \leq i < j \leq n,$$

i.e. on the skew symmetric matrix

$$Z = pq^T - qp^T$$

of order n^2 , a benefit of including the term $\text{trace}^2(P^T Q)$. Indeed, we have

$$\|Z\|^2 = 2 \left(\|P\|^2 \|Q\|^2 - \text{trace}^2(P^T Q) \right),$$

and all entries of the commutator $[P, Q]$ obviously are linear forms of the $z_{i,j}$ -s.

Let us formulate the primal and dual semi-definite programming problems (see e.g. in [8]) for the eigenvalue optimization:

$$\min \{ \text{tr}(CX) : X \geq 0, \text{tr}(A_i X) = 0, 1 \leq i \leq M, \text{tr}(X) = 1 \} \quad (\text{Primal})$$

$$\max \{ y_{M+1} : S \equiv C - \sum_{t=1}^M y_t A_t - y_{M+1} I \geq 0 \} \quad (\text{Dual})$$

where C, S, X, A_t and the identity $I = I_N$ are all real symmetric N th order matrices, C and $(A_t)_1^M$ are given, the primal matrix X , the dual (slack) matrix S and vector y are the solutions of the program, $\text{tr}(AB) \equiv \text{trace}(AB)$ denotes the scalar product of the symmetric matrices A and B , and \geq stands for the semi-definite ordering: $A \geq B$ iff $A - B$ is positive semi-definite.

The quantities $z_{i,j}$ will play the role of 'candidate monomials' (better to say, differences, and hereafter called candidates) with ordering

$$z = (z_{1,2}, z_{1,3}, z_{2,3}, z_{1,4}, \dots, z_{1,n}, \dots, z_{n-1,n})^T.$$

The indices can be read from the "big" index matrix

$$\text{POS} = \begin{pmatrix} 0 & 1 & 2 & 4 & 7 & \dots \\ \cdot & 0 & 3 & 5 & 8 & \dots \\ \cdot & \cdot & 0 & 6 & 9 & \dots \\ \cdot & \cdot & \cdot & 0 & 10 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

of order n^2 to be

$$(i, j) \sim k \equiv i + \frac{(j-1)(j-2)}{2}, \quad 1 \leq i < j \leq n^2.$$

Note that $z_{i,i} = 0$ for all i , and that the entries below the diagonal are omitted due to $z_{i,j} = -z_{j,i}$, enabling us to reduce the number of unknowns. Also note that IND is related to P and Q , while POS is connected with Z .

As an example, we give the biquadratic form BW as a quadratic form of the quantities $(z_{i,j})$ for $n = 3$. Observe that $\|Z\|^2 = \|Z\|_F^2 = 2 \sum_{1 \leq i < j \leq 9} z_{i,j}^2$.

Example 1. For $n = 3$ the objective takes the form

$$\begin{aligned} BW &= \|Z\|^2 - (z_{2,4} + z_{3,7})^2 - (z_{1,2} + z_{2,5} + z_{3,8})^2 - (z_{1,3} + z_{2,6} + z_{3,9})^2 \\ &- (-z_{1,4} - z_{4,5} + z_{6,7})^2 - (-z_{2,4} + z_{6,8})^2 - (-z_{3,4} + z_{5,6} + z_{6,9})^2 \\ &- (-z_{1,7} - z_{4,8} - z_{7,9})^2 - (-z_{2,7} - z_{5,8} - z_{8,9})^2 - (-z_{3,7} + z_{6,8})^2. \end{aligned}$$

(Note that the form BW can be thought of as a function of the matrices (P, Q) , the vectors (p, q) , the matrix Z , or of the vector z .) We give now all the (quadratic) relations holding for the variables $(z_{i,j})_{1 \leq i < j \leq n^2}$ as

$$z_{i,j} z_{k,l} + z_{i,l} z_{j,k} - z_{i,k} z_{j,l} = 0, \quad 1 \leq i < j < k < l \leq n^2. \quad (2)$$

These easily checked relations define $M = \binom{n^2}{4}$ symmetric constraint matrices A_t , each having exactly 6 nonzero (off-diagonal) entries. For instance, equation

$$z_{2,3} z_{4,5} + z_{2,5} z_{3,4} - z_{2,4} z_{3,5} = 0$$

defines an A_t with nonzero entries in positions $(3, 10)$, $(8, 6)$, $(5, 9)$ and their transposes, see the matrix POS. Now we can state our main theorem.

Theorem 1 *The minimum value of γ_n , for which (1) is a sum of squares is*

$$\gamma_n = \frac{n-2}{2}.$$

Proof. We give the optimal primal and dual solutions and describe the main characteristics of the optimal dual matrix. Since the objectives coincide, the strong duality theorem yields the desired result.

By fixing the order of the variables $(z_{i,j})$ above, matrix C is uniquely determined. To get the (slack) matrix $S = C - \sum y_t A_t$, we use the following strategy. Note that we not only give the set (A_t) of active constraints (as e.g. when taking the half Newton-polytope), but also give their coefficients (y_t) .

Strategy A. Assume the commutator $[P, Q]$ contains an entry $(z_{i,j} + z_{k,l} + \dots)$ with i, j, k, l distinct and $i < j, k < l$. Then the quadratic form $z^T C z$ associated with C necessarily contains a term $2 z_{i,j} z_{k,l}$. We 'halve' this term, and leave one $z_{i,j} z_{k,l}$ unchanged as is, while apply for the other term the basic quadratic relation (2). By using the correct sign, this defines a constraint A_t and the corresponding dual variable y_t for some t . Finally, let $y_{m+1} = -\frac{n-2}{2}$.

Now we give the obtained primal and dual solutions. In view of the quite combinatorial character of the problem, we do not detail each block, instead we give some explanations and important cross-references (control sums) and for matrix S we provide Table 1. with all essential informations.

The Primal Problem

Before defining the optimal primal matrix X , we note that its rank is $\binom{n}{2}$. For indices $(i, j) : 1 \leq i < j \leq n$ we define the vectors $v_{i,j}$ of dimension $\binom{n^2}{2}$

to have $4(n-1)$ nonzero coordinates (four 2's and $4(n-2) \pm 1$'s) using row_i , row_j , column_i and column_j of the index matrix IND, cf. Example 2 below.

Next we form the matrix of these vectors

$$V = [v_{1,2}, v_{1,3}, v_{2,3}, \dots, v_{n-1,n}],$$

and define matrix $X_0 = VV^T = \sum v_{i,j}v_{i,j}^T$ with the following properties:

X_0 is a symmetric matrix of order $N = \binom{n^2}{2}$ and rank $\binom{n}{2}$. The $v'_{i,j}$'s are orthogonal with norm square $\|v_{i,j}\|^2 = 4 \cdot 4 + 4(n-2) \cdot 1 = 4(n+2)$. The trace of X_0 is

$$\text{tr}(X_0) = \sum_{i < j} \text{tr}(v_{i,j}v_{i,j}^T) = \sum_{i < j} \|v_{i,j}\|^2 = 4(n+2) \binom{n}{2},$$

thus by defining

$$X = \left(4(n+2) \binom{n}{2}\right)^{-1} X_0$$

we get a trace 1 matrix. The eigenvalues of X_0 are $4(n+2)$, those of X are $\binom{n}{2}^{-1}$ (hence $\binom{n}{2}^{-1}X$ is a projection). The $v_{i,j}$'s are also eigenvectors of C :

$$C v_{i,j} = (2-n)/2 v_{i,j}.$$

Furthermore we have

$$\text{tr}(CX_0) = \sum_{i < j} \text{tr}(C v_{i,j}v_{i,j}^T) = \sum_{i < j} v_{i,j}^T C v_{i,j} = \frac{2-n}{2} \sum_{i < j} \|v_{i,j}\|^2,$$

and finally, the primal objective equals

$$\text{tr}(CX) = \frac{\text{tr}(CX_0)}{\text{tr}(X_0)} = \frac{2-n}{2}. \quad (3)$$

The Dual Problem

The matrix $S = C - \sum y_t A_t$ resulting from Strategy A is positive semi-definite and decomposes into some blocks given in Table 1. (Observe that all eigenvalues and diagonal entries of $2S$ are integer – a reason for the factor 2.)

Here we list the important facts and control sums concerning the blocks of S , and in Example (3) we give further hints for understanding the construction.

ROW-control: an element in the last column of row i is the scalar product of row 1 and row i . For instance, the number of zero eigenvalues—the defect of S —equals to $\binom{n}{2}2 + 1(n-1) = n^2 - 1$.

1	No of blocks	$\binom{n}{2}$	1	$3\binom{n}{4}$	$\binom{n}{2}$	Total
2	Block sizes	$6n-8$	$\binom{n}{2}$	4	1	
3	Eig=0	2	$n-1$	—	—	n^2-1
4	Eig=4	1	—	—	—	$n(n-1)/2$
5	Eig=n	$2n-4$	$\binom{n-1}{2}$	1	—	$(n^2-1)(n-2)(n+4)/8$
6	Eig=n+2	$3n-5$	—	2	2	$(n^2-1)(n-2)(n+4)/4$
7	Eig=n+4	$n-3$	—	1	—	$n(n-1)(n^2+n-2)/8$
8	Eig=2n+2	1	—	—	—	$n(n-2)/2$
9	Diag	$n(+2)$	$n-2$	$n+2$	$n+2$	$(n^3-n)(n^2+2n-4)/2$

Table 1: Decomposition of the matrix "2S"

EIG-control: the last column (the number of eigenvalues, rows 3 to 8) sums up to $\binom{n^2}{2}$, the order of the matrix 2S.

DIAG-control: The sum of the elementwise products of row 1, 2 and 9,

$$\binom{n}{2} \left(2n * n + 4(n-2)(n+2) \right) + 1 \binom{n}{2} (n-2) + 3 \binom{n}{4} 4(n+2) + \binom{n}{2} 1(n+2)$$

equals to $\binom{n}{2} (n+1)(n^2+2n-4)$, the trace of 2S. (In the blocks of order $6n-8$ there are $2n$ diagonal elements "n", and $4(n-2)$ diagonal elements "(n+2)".)

TRACE-control: the trace of the coefficient matrix C equals

$$\text{tr}(C) = 2 \binom{n^2}{2} - n(n-1) - (n^2-n)n = n(n-1)^2(n+1).$$

The first subtrahend comes from the diagonal of the commutator [P, Q], the second from their off-diagonal elements. Due to $\text{diag}(S) = \text{diag}(C) + \gamma_n I$, the connection between the traces of matrices C and S is

$$\text{tr}(2S) = 2 \left(\text{tr}(C) + \frac{n-2}{2} \binom{n^2}{2} \right).$$

The number of all constraints is $\binom{n^2}{4}$, while that of active constraints equals

$$n \binom{n-1}{2} + n(n-1) \left(\binom{n-2}{2} + 2(n-2) \right) = \binom{n}{2} (n^2-4) \equiv 3(n+2) \binom{n}{3}.$$

Here the first term is associated with the main diagonal of $R \equiv [P, Q]$ (by virtue of $z_{i,i} = 0$ there are only $n-1$ terms in $R(i, i)$), while the rest comes

from the off-diagonal of the commutator R (where there always are two terms for which the basic relations do not apply, see the Example 2).

Thus S is positive semi-definite with defect $n^2 - 1$, and its eigenvalues range in the interval $[0, n + 1]$. To sum up, the primal objective (3) coincides with the dual objective y_{M+1} , the negative of γ_n , which proves the theorem. \square

There holds no strict complementarity, for $\text{rank}(X) = \binom{n}{2} < n^2 - 1 = \text{def}(S)$.

Example 2 To define the primal matrix X take the four scalar products

$$\langle \text{row}_i, \text{col}_j \rangle, \quad \langle \text{col}_i, \text{row}_j \rangle, \quad \langle \text{row}_i, \text{row}_j \rangle, \quad \langle \text{col}_i, \text{col}_j \rangle$$

in the index matrix IND where each of the four products determine n coordinates in $v_{i,j}$ as follows. If $n = 3$ and $i = 1, j = 2$, then $\text{row}_1 = [1, 2, 3]$, $\text{col}_2 = [2, 5, 8]^T$ which yields by $(1, 2) \sim 1, (2, 5) \sim 8, (3, 8) \sim 24$ the coordinates 1, 8, 24, see also matrix POS . Similarly we calculate the other three triples, giving together

$$1, 8, 24; 4, 10, 21 (!); 4, 8, 13; 1, 10, 28.$$

The repeated elements $(1, 4, 8, 10)$ denote positions with value 2. The exclamation sign refers to an entry -1 (since $(7, 6)$ must be inverted to $(6, 7) \sim 21$). To sum up, we get

$$v_{1,2} = (2, 0, 0, 2, 0, 0, 0, 2, 0, 2, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T.$$

Example 3 Hints for obtaining the dual matrix. We give some details for the $\binom{n}{2}$ most important blocks of order $6n - 8$. There is a one-to-one correspondence between these blocks and ordered pairs (i, j) , $1 \leq i < j \leq n$. To collect the indices for the block containing $z_{i,j}$, we have to consider the $4(n - 1)$ terms in

$$\langle \text{row}_i, \text{col}_j \rangle, \quad \langle \text{col}_i, \text{row}_j \rangle, \quad \langle \text{row}_i, \text{row}_j \rangle, \quad \langle \text{col}_i, \text{col}_j \rangle$$

(the same as for $v_{i,j}$ above!) and further $2(n - 2)$ terms in the products

$$IND(i, j) * \text{diag}(\neq i, j), \quad IND(j, i) * \text{diag}(\neq i, j).$$

Here $\text{diag}(\neq i, j)$ stands for the $n - 2$ entries of the diagonal of IND , differing from i, j . As in Example 2, choosing $n = 3, i = 1, j = 2$, vector $\text{diag}(\neq 1, 2)$ reduces to the $(3, 3)$ entry 9, thus we get (using index matrices IND and POS)

$$((1, 2), (3, 3)) \sim (2, 9) \sim 30 \quad \text{and} \quad ((2, 1), (3, 3)) \sim (4, 9) \sim 32.$$

Hence the diagonal block containing row 1 (related to $z_{1,2}$) also contains rows 30 and 32. The whole index set at issue is $[1, 4, 8, 10, 13, 21, 24, 28, 30, 32]$, and the corresponding block is the 10×10 (irreducible) matrix

$$\begin{pmatrix} 3 & 0 & -2 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 3 & 0 & -2 & 0 & 1 & 0 & -1 & 0 & 0 \\ -2 & 0 & 3 & 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & -2 & 0 & 3 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & -1 & 5 & 0 & 0 & -1 & -1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 3 & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & 0 & 0 & -1 & 3 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 0 & 0 & 5 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 5 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 5 \end{pmatrix}$$

with eigenvalues $(0, 0, 3, 3, 4, 5, 5, 5, 5, 8)$.

3 Tridiagonal (and backward tridiagonal) matrices

In a former paper [4] we have shown that for n th order matrices P, Q with only nonzero entries in row 1 and column n the BW form is sos, however in case of (additional) main diagonal elements this is no more true. Therefore one would guess that $3n + O(1)$ nonzero elements cannot be allowed, however the result below shows that the answer depends on the position of these elements.

We shall use an index matrix given e.g. for $n = 3$ as $\text{IND} = \begin{pmatrix} 1 & 2 & 0 \\ 3 & 4 & 5 \\ 0 & 6 & 7 \end{pmatrix}$.

Lemma 4 *For tridiagonal P, Q the BW form is sos, especially we have*

$$\begin{aligned} \text{BW} &= 2 \sum_{i < j} z_{i,j}^2 \\ &- \sum (z_{3i-4,3i-3} - z_{3i-1,3i})^2 - \sum z_{3i-2,3i-1}^2 - \sum z_{3i,3i+3}^2 \\ &- \sum (z_{3i-2,3i-1} + z_{3i-1,3i+1})^2 - \sum (z_{3i-2,3i} + z_{3i,3i+1})^2 \\ &= \sum (z_{3i-4,3i-1} + z_{3i-3,3i})^2 + (z_{3i-4,3i} - z_{3i-3,3i-1})^2 \\ &+ \sum (z_{3i-2,3i-1} - z_{3i-1,3i+1})^2 + \sum (z_{3i-2,3i} - z_{3i,3i+1})^2 \\ &+ \sum z_{3i,3i+2}^2 + 2 \sum z_{3i-2,3i+1}^2 + 2 \sum_{i+5 \leq j} z_{i,j}^2 - \sum z_{3i-1,3i+3}^2. \end{aligned}$$

Remark 5 *The first equality gives the biquadratic form at issue, the second one is the claim: the sum of squares representation. (The negative terms in the last row are evidently canceled.)*

n	$\lambda = 0$	$\lambda = 1$	$\lambda = 2$	$\lambda = 3$	2-bl.	act.	$\text{rk}(X)$
2	3	0	3	0	2	0	3
3	7	1	12	1	6	1	7
4	11	2	30	2	10	2	11
5	15	3	57	3	14	3	15
6	19	4	93	4	18	4	19
7	23	5	138	5	22	5	23
8	27	6	192	6	26	6	27

Table 2: “Tridiagonal matrices”

Although SDP is not needed here, for the identity of the Lemma can be proved directly, we yet give some facts. The eigenvalues of the dual matrix S for the actual semidefinite programming problem are integers $(0, 1, 2, 3)$ in this case, too. This is so because matrix S decomposes into at most second order blocks of the form $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ and $\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$.

Table 2 illustrates the main features of the underlying semidefinite program. First the number of the eigenvalues of S are given, then the number of 2×2 blocks in S (the number of scalar blocks is not shown), the number of the active ($y_i \neq 0$) constraints, and finally, the rank of X . (The $n - 2$ active constraints correspond to the positions $(i - 1, i)$, $(i, i - 1)$, $(i, i + 1)$ and $(i + 1, i)$ in IND.)

It is easy to get a formula for these quantities, e.g. the number of eigenvalues $\lambda_i = 2$ can be determined by subtracting the number of all other eigenvalues from the order $(3n - 2)(3n - 3)/2$ of S . The result is $3 + 9\binom{n-1}{2}$.

Note that strict complementarity does hold: the number of zero eigenvalues of S coincides with $\text{rank}(X)$, the number of nonzero eigenvalues of X .

Backward tridiagonal matrices

They have many similar properties, except that the case n odd is worse: while for n even all the eigenvalues of S are integers (lying in $[0, 4]$), for n odd this does not hold, therefore we write ‘-’ instead. Also, in this case there are (apart from the scalar and 2×2 blocks) 4×4 blocks, too. All this information is contained in Table 3 from where one can see that for n even we again have strict complementarity, as in the tridiagonal case.

n	$\lambda = 0$	$\lambda = 1$	$\lambda = 2$	$\lambda = 3$	$\lambda = 4$	act	2-bl.	4-bl.	rk(X)
2	3	0	3	0	0	2	0	0	3
3	8	-	-	-	-	3	3	7	5
4	13	4	25	0	3	6	3	8	13
5	20	-	-	-	-	11	6	17	18
6	25	6	81	2	6	14	6	18	25
7	32	-	-	-	-	30	9	27	30
8	37	8	173	4	9	22	9	28	37

Table 3: "Backward tridiagonal matrices"

Example 6 We calculate the number act of active constraints:

$$\text{act} = \begin{cases} 5n - 12, & n \text{ even} \\ 5n - 8, & n \text{ odd} \end{cases}$$

The number of terms in a typical row of the product of backward tridiagonal matrices usually equals $(0, \dots, 0, 1, 2, 3, 2, 1, 0, \dots, 0)$. However, in case of the commutator $PQ - QP$ there are some minor changes: for odd order 1, for even order 2 main diagonal entries contain only two terms (instead of 3), due to the identity $z_{i,j} + z_{j,i} = 0$. On the other hand, if n is even, there are two opposite entries (with indices $(k, k+1)$ and $(k+1, k)$, where $k = n/2$) which do not generate any constraint, for the corresponding indices are not distinct.

Now we easily calculate the number asked, which is e.g. for $n = 6$ equal to $5n - 12 = 18$. To this consider the matrix

$$\begin{pmatrix} 2 & 2 & 1 & 0 & 0 & 0 \\ 2 & 3 & 2 & 1 & 0 & 0 \\ 1 & 2 & 2 & * & 1 & 0 \\ 0 & 1 & * & 2 & 2 & 1 \\ 0 & 0 & 1 & 2 & 3 & 2 \\ 0 & 0 & 0 & 1 & 2 & 2 \end{pmatrix}$$

with the number of terms in a given position of $[P, Q]$, and take $\binom{e}{2}$ for any entry $e > 1$. They sum up to $2 * \left(6\binom{2}{2} + \binom{3}{2}\right) = 18$. The general case is similar.

4 Cyclic Hankel matrices

When investigating Hankel matrices, we find that – except for the case $n = 3$, see below – they do not generate sos BW forms. However, cyclic ones behave well. We make use of the small index matrix (given for $n = 3$): $\text{IND} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \\ 3 & 1 & 2 \end{pmatrix}$.

Theorem 7 *For cyclic Hankel matrices P, Q the BW form is a sum of squares.*

Proof. Using the above-defined index matrix with $(1, 2, \dots, n)$ as first row and $(n, 1, \dots, n-1)^T$ as last column, we obtain

$$\|P\|^2 = n\|p\|^2, \quad \|Q\|^2 = n\|q\|^2, \quad \text{trace}(P^T Q) = np^T q,$$

consequently

$$2 \left(\|P\|^2 \|Q\|^2 - \text{trace}^2(P^T Q) \right) = 2n^2 (\|p\|^2 \|q\|^2 - (p^T q)^2).$$

The commutator $[P, Q]$ is a skew symmetric cyclic Toeplitz matrix having

$$k = k_n = \left\lfloor \frac{n-1}{2} \right\rfloor$$

different entries $t_i = t_i^{(n)}$ with row one as

$$\begin{aligned} (0, t_1, \dots, t_k, -t_k, \dots, -t_1) & \quad (n \text{ odd}) \\ (0, t_1, \dots, t_k, 0, -t_k, \dots, -t_1) & \quad (n \text{ even}). \end{aligned}$$

Thus the subtrahend is $\|R\|^2 = 2n \sum t_i^2$, and the whole BW form equals

$$2n \left(n \sum_{i < j} z_{i,j}^2 - \sum_1^k t_i^2 \right).$$

Observe now that all terms in

$$t_i = t_i^{(n)} = \sum_{j=1}^{n-i} z_{j,i+j} - \sum_{j=1}^i z_{j,n-i+j}$$

are distinct ($i = 1, \dots, k$), hence the Cauchy-Schwarz inequality in conjunction with $nk = n \left\lfloor \frac{n-1}{2} \right\rfloor \leq \binom{n}{2}$ imply

$$\sum_{i=1}^k t_i^2 \leq \sum_{i=1}^k n \left(\sum_{j=1}^{n-i} z_{j,i+j}^2 + \sum_{j=1}^i z_{j,n-i+j}^2 \right) \leq n \sum_{i < j} z_{i,j}^2,$$

which proves the theorem. The last inequality turns into equality for n odd.

□

Remark 8 The case $n = 4$ is especially interesting. Then the commutator is

$$\begin{pmatrix} 0 & t & 0 & -t \\ -t & 0 & t & 0 \\ 0 & -t & 0 & t \\ t & 0 & -t & 0 \end{pmatrix}$$

with $t = t_1 = t_1^{(4)} = z_{1,2} + z_{2,3} + z_{3,4} - z_{1,4}$, therefore the formula

$$\begin{aligned} & 4(z_{1,2}^2 + z_{1,3}^2 + z_{2,3}^2 + z_{1,4}^2 + z_{2,4}^2 + z_{3,4}^2) = \\ & + (z_{1,2} + z_{2,3} - z_{1,4} + z_{3,4})^2 + (z_{1,2} - z_{2,3} + z_{1,4} + z_{3,4})^2 \\ & + (z_{1,2} + z_{1,3} - z_{2,4} - z_{3,4})^2 + (z_{1,2} - z_{1,3} + z_{2,4} - z_{3,4})^2 \\ & + (z_{1,3} + z_{2,3} + z_{1,4} + z_{2,4})^2 + (z_{1,3} - z_{2,3} - z_{1,4} + z_{2,4})^2, \end{aligned}$$

(a consequence of Eulers identity) yields the sos-representation needed.

Example 9 The case of (general) third order Hankel matrices. The index matrix IND is now $\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \end{pmatrix}$, the order of C , S and the constraint matrices $\{A_t\}$ is $\binom{5}{2} = 10$, the number of the A_t -s is $\binom{5}{4} = 5$. By help of vector

$$z = (z_{1,2}, z_{1,3}, z_{2,3}, z_{1,4}, z_{2,4}, z_{3,4}, z_{1,5}, z_{2,5}, z_{3,5}, z_{4,5})^T$$

and matrix C the objective can be written as $BW = z^T C z = \text{tr}(C z z^T)$, which becomes – by means of a standard SDP relaxation – $\text{trace}(CX)$. Our MATLAB program yields $y = (0, 0, 1, 0, 0, 0)$, i.e. only one constraint will be active, giving

$$S = C - y_3 A_3 = \begin{pmatrix} 1 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & \{1\} \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 4 & 0 & 0 & -2 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & \{-1\} & 0 & 0 \\ 0 & -1 & 0 & 0 & 3 & 0 & \{1\} & 0 & -1 & 0 \\ -1 & 0 & -2 & 0 & 0 & 4 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & \{1\} & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \{-1\} & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 2 & 0 \\ \{1\} & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

(In the original C the six entries in braces are zero.) The last zero in y indicates the sos representability. To obtain the concrete sos form, we calculated the

eigen-decomposition of the three blocks

$$B_1 = \begin{pmatrix} 1 & -1 & -1 & 1 \\ -1 & 4 & -2 & -1 \\ -1 & -2 & 4 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}, B_2 = \begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 3 & 1 & -1 \\ 0 & 1 & 1 & 0 \\ -1 & -1 & 0 & 2 \end{pmatrix}, B_3 = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

with integer eigenvalues

$$E_1 : \begin{pmatrix} 0 & 0 & 4 & 6 \end{pmatrix}, \quad E_2 : \begin{pmatrix} 0 & 1 & 3 & 4 \end{pmatrix}, \quad E_3 : \begin{pmatrix} 1 & 3 \end{pmatrix}$$

and (unnormalized, integer, columnwise) eigenvectors

$$V_1 : \begin{pmatrix} 2 & -1 & 1 & 0 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 0 & 3 & 1 & 0 \end{pmatrix}, \quad V_2 : \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & -3 \\ -1 & 2 & 0 & -1 \\ 1 & 1 & -1 & 1 \end{pmatrix}, \quad V_3 : \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We sum up the result: with $z_{i,j} = p_i q_j - q_i p_j$, $1 \leq i < j \leq 5$ the following identity holds for the BW form generated by two third order Hankel matrices:

$$\begin{aligned} & 2z_{1,2}^2 + 3z_{1,3}^2 + 6z_{2,3}^2 + 2z_{1,4}^2 + 4z_{2,4}^2 + 6z_{3,4}^2 + z_{1,5}^2 + 2z_{2,5}^2 + 3z_{3,5}^2 + 2z_{4,5}^2 \\ & - (z_{1,3} + z_{2,4} + z_{3,5})^2 - (z_{1,2} + z_{2,3} + z_{3,4})^2 - (z_{2,3} + z_{3,4} + z_{4,5})^2 = \\ & (z_{1,2} - z_{2,3} - z_{3,4} + z_{4,5})^2 + 3(z_{2,3} - z_{3,4})^2 \\ & + \frac{1}{6}(z_{1,3} + 2z_{1,5} + z_{3,5})^2 + \frac{3}{2}(z_{1,3} - z_{3,5})^2 + \frac{1}{3}(z_{1,3} - 3z_{2,4} - z_{1,5} + z_{3,5})^2 \\ & + \frac{1}{2}(z_{1,4} + z_{2,5})^2 + \frac{3}{2}(z_{1,4} - z_{2,5})^2. \end{aligned}$$

5 Toeplitz matrices

In this section P and Q will be arbitrary real Toeplitz matrices. Observe that the main diagonal entries don't play any role (to prove this use temporarily the more standard notation $P = (p_{j-i})$ and $Q = (q_{j-i})$, then the (i, j) entry in $R = [P, Q]$ equals $\sum z_{k-i, j-k}$, while $z_{0, j-i} + z_{j-i, 0} = 0$). Hence we can reduce the number of variables to get e.g. for $n = 3$ the index matrix $IND = \begin{pmatrix} 0 & 1 & 2 \\ 3 & 0 & 1 \\ 4 & 3 & 0 \end{pmatrix}$.

Another speciality is that now there occur repeated terms as well. To handle these, introduce the multiplicity vector μ of dimension m by

$$\mu_i = \{\text{the number of occurrences of } p_i \text{ in } P, \ 1 \leq i \leq m\}.$$

Then the following easily proved representation holds.

Lemma 10

$$2 \left(\|P\|^2 \|Q\|^2 - \text{trace}^2(P^T Q) \right) = 2 \sum_{i=1}^{m-1} \sum_{j=i+1}^m \mu_i \mu_j z_{i,j}^2,$$

and (since the commutator is skew persymmetric), $\|R\|^2 = 2 \sum_{i=1}^2 \sum_{j=1}^{n-i} r_{i,j}^2$.

In view of the lemma, we define the symmetric matrix C by help of equation $z^T C z = \frac{1}{2} BW(p, q)$. Then there are $m = 2(n-1)$ possible nonzero elements, the candidate vector z has dimension $N = \binom{m}{2}$, and the total number of constraints (A_t) is $M = \binom{m}{4}$. For this problem we formulate a 'quasi-optimal' strategy of choosing the dual variables.

Strategy B. Since the entries of $[P, Q]$ are linear forms in $(z_{i,j})$, their squares figuring in $\|R\|^2$ involve some mixed products of the form $\pm 2 z_{i,j} z_{k,l}$. Whenever finding such a term with distinct $\{i, j, k, l\}$, we increase the actual value of y .

It turns out that Strategy B works for n , $3 \leq n \leq 7$, however, for $n \geq 8$ the dual matrix $S = C - \sum y_t A_t$ will have (more and more) negative eigenvalues.

Lemma 11 *For orders n not exceeding 7, the matrix S is p.s.d, i.e. for these values the BW form is sos. Some further properties of S of arbitrary order n are: the minimum off-diagonal entry of S is $-\lfloor \frac{n-1}{2} \rfloor$; the defect of S , i.e. the multiplicity of zero as eigenvalue is $n-1$; the maximal diagonal entry and also the maximal eigenvalue is $n(n-2)$. Moreover, S is a direct sum of two types of submatrices of the following order:*

- type (a): $2, 4, 6, \dots, 2(n-2)$; (denote by B the largest block here)
- type (b): $1, 1, 2, 2, \dots, n-2, n-2, n-1$.

The orders of these matrices sum up to $(n-1)(2n-3)$, the order of S .

The largest block B of type (a) is crucial. It has a decomposition $B = \begin{pmatrix} D & H \\ H & D \end{pmatrix}$, with D diagonal, H Hermitian (i.e. symmetric), both of order $n-2$. The diagonal elements of D are $(i(i+1))$ in reverse order: $((n-2)(n-1), \dots, 6, 2)$. Matrix H is also of a special structure: the elements on the border are -1 , those on the 'neighboring' border are -2 , and so on. This matrix is p.s.d. for $n \leq 7$, but has at least one negative eigenvalue for $n \geq 8$.

Remark 12 *The further submatrices of type (a) also are critical, e.g. the next one (of order $2(n-3)$) has a similar form with diagonal elements $(i(i+2))$ in D , while H is the same (of the appropriate size). Therefore there is a second negative eigenvalue for n , $14 \leq n \leq 20$, and so on. In general, the symmetric matrices H are of the same form, and the diagonal entries of D are $(i(i+k))_i$.*

Example 13 *Matrices of order 5. In this case P and Q have $m = 2(n-1) = 8$ nonzero elements, the candidate vector z has dimension $\binom{m}{2} = 28$, the total number of constraints is $\binom{m}{4} = 70$, and the number of active constraints is 14.*

It always suffices to examine the first row and the first column of R , for all other entries are contained in these, e.g. $R(1,1) = z_{1,5} + z_{2,6} + z_{3,7} + z_{4,8}$, and $R(2,2) = z_{2,6} + z_{3,7}$. The number of the active constraints for $n = 5$, coming from row 1 and column 1 is indeed $6 + 2(3 + 1) = 14$, as stated above. This can be proved by induction, by noting that

$$\binom{n-1}{2} + 2\left\{\binom{n-2}{2} + \binom{n-3}{2} + \cdots + \binom{2}{2}\right\} = \frac{1}{6}(n-1)(n-2)(2n-3).$$

As regards the y coordinates, since the product $2z_{2,6}z_{3,7}$ occurs two times (as the above formulae show), we write -2 in the suitable positions (overwriting the -1 -s) to get $S(13,17) = S(3,21) = -2$, and so on.

Now we give another example illustrating the role of the crucial block B .

Example 14 *The case $n = 8$. The matrices D and H are now:*

$$D = \begin{pmatrix} 42 & 0 & 0 & 0 & 0 & 0 \\ 0 & 30 & 0 & 0 & 0 & 0 \\ 0 & 0 & 20 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}, \quad H = \begin{pmatrix} -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -2 & -2 & -2 & -2 & -1 \\ -1 & -2 & -3 & -3 & -2 & -1 \\ -1 & -2 & -3 & -3 & -2 & -1 \\ -1 & -2 & -2 & -2 & -2 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}.$$

The characteristic polynomial of the block $B = \begin{pmatrix} D & H \\ H & D \end{pmatrix}$ factorizes into $p_1 p_2$, where $p_1(x) = x^6 - 100x^5 + 536x^4 - 53472x^3 + 327472x^2 - 575680x - 145152$, and p_1 has a negative zero: -0.2228 . (All other zeroes of p_1 and p_2 are positive.)

Finally we mention that although the above strategy works only up to $n = 7$, the standard semidefinite program yields results indicating that BW can be sos for some larger orders, too, hence we guess that BW is sos in general. The difficulty is that the corresponding dual variables (y_t) of the program are not recognizable real numbers. Nevertheless we formulate the following.

Conjecture 15 *The Böttcher-Wenzel form (1) generated by two real Toeplitz matrices is sos, i.e. a sum of squares of polynomials, now: quadratic forms. Give – if possible – a rational certification, i.e. rational parameters (y_t) such that $S = C - \sum y_t A_t$ is positive semidefinite.*

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